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Title: Preparation of Nuclear Data Libraries for Web Release, Tutorial for Generating Correlated Random Samples and Propagation of Uncertainty

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Conlin, Jeremy Lloyd
Parsons, Donald Kent

Intended for: Presentation to Group
Report

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Los Alamos NATIONAL LABORATORY

Preparation of Nuclear Data Libraries for Web Release

Ryan Siggins, Jeremy Conlin

August 4, 2021

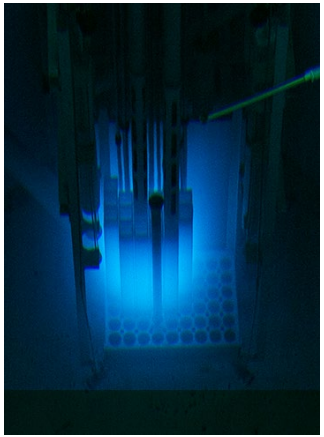
Tutorial for Generating Correlated Random Samples and Propagation of Uncertainty

Ryan Siggins, Kent Parsons

August 4, 2021

About me

- Graduated with a BS in Nuclear Engineering from Missouri S&T
- Returning this fall to begin work on Master's in Nuclear Engineering
- Work with campus EHS as HP Tech



More about me!

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Preparation of Nuclear Data Libraries for Web Release

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Previous Releases of MCNP

- MCNP6.2 Released in 2018 in 3 DVDs
  - 1 DVD with MCNP, 2 DVDs with all nuclear data up to *ENDF/B-VII.1*
    - Up to and including the *ENDF71x* and *ENDF71SaB* libraries
    - Constitutes ~60 GB of uncompressed nuclear data

- Release of MCNP6.3
  - Adding *Lib80x, ENDF80SaB2,* and *CP2020* libraries
    - Another ~42 GB of data in those libraries alone

- More detailed libraries will only get larger in the future

Why distribute via DVD?

- For a while, it was the easiest way to do it
  - MCNP had to be shipped because it was controlled, so sent a few more disks with the data
  - Shipping ALL the previous nuclear data ensures users who may need it have it

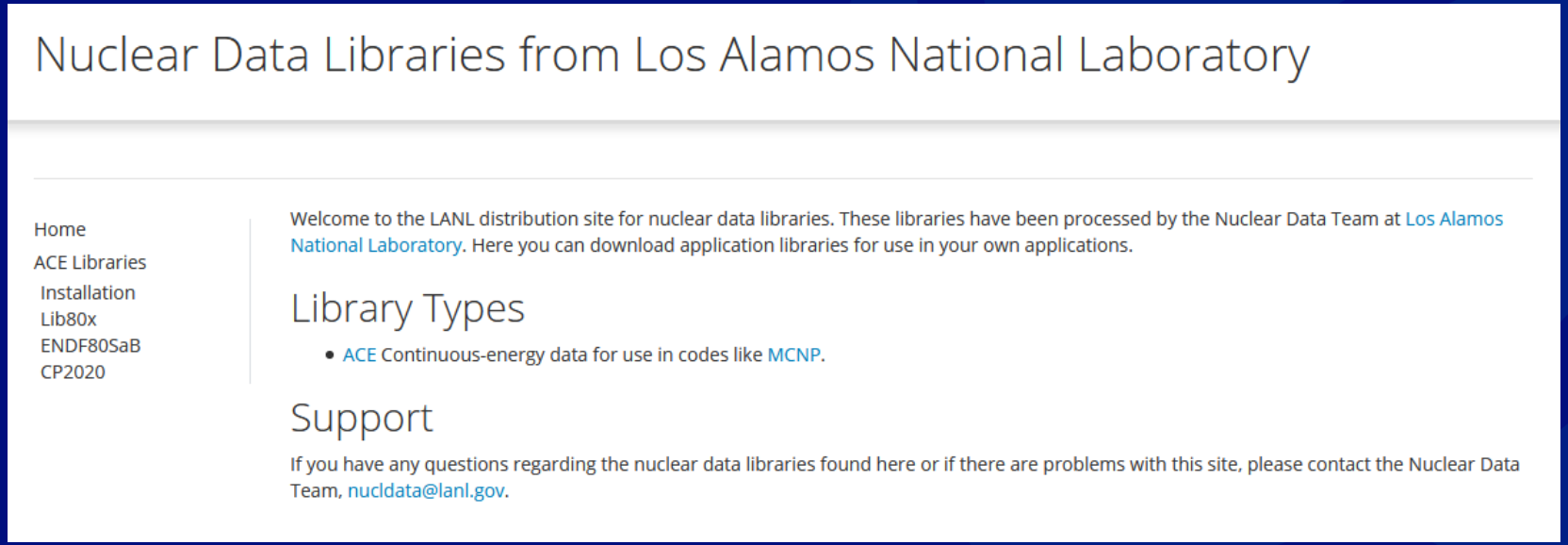
- However, this method is flawed in a few ways
  - Nuclear data is public, so treating it as controlled restricts user access to new data
    - *ENDF/B-VIII.0* had 2 sets of ACE files released the **same year** as MCNP6.2, but couldn't be included
  - Outdated
  - Many modern computers don't include a DVD reader

Web Hosted Nuclear Data

- Move distribution of nuclear data to online platform
  - It's 2021
  - More frequent nuclear data updates
  - Greater ease of acquiring nuclear data
  - User flexibility in what nuclear data to download

Web hosted nuclear data

nucleardata.lanl.gov

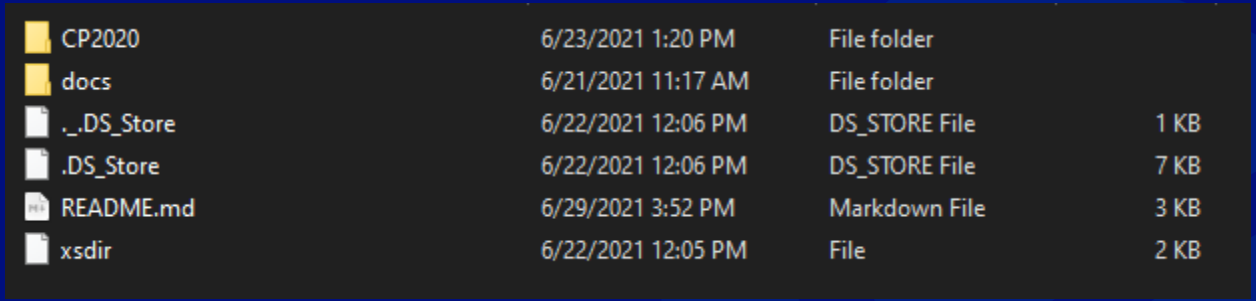


Library Management and Tools

Data

Documentation

Markdown Summary

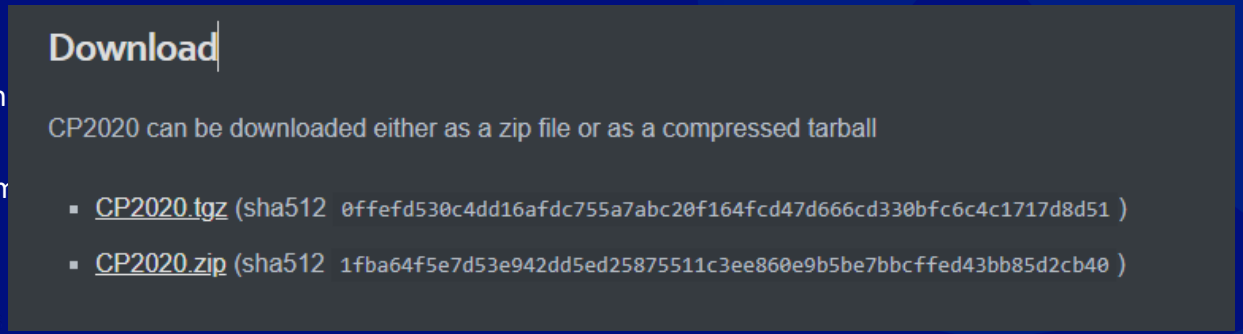


CP2020	6/23/2021 1:20 PM	File folder	
docs	6/21/2021 11:17 AM	File folder	
._.DS_Store	6/22/2021 12:06 PM	DS_STORE File	1 KB
.DS_Store	6/22/2021 12:06 PM	DS_STORE File	7 KB
README.md	6/29/2021 3:52 PM	Markdown File	3 KB
xsdir	6/22/2021 12:05 PM	File	2 KB

Move_and_shasum.sh

Markdown

Docum



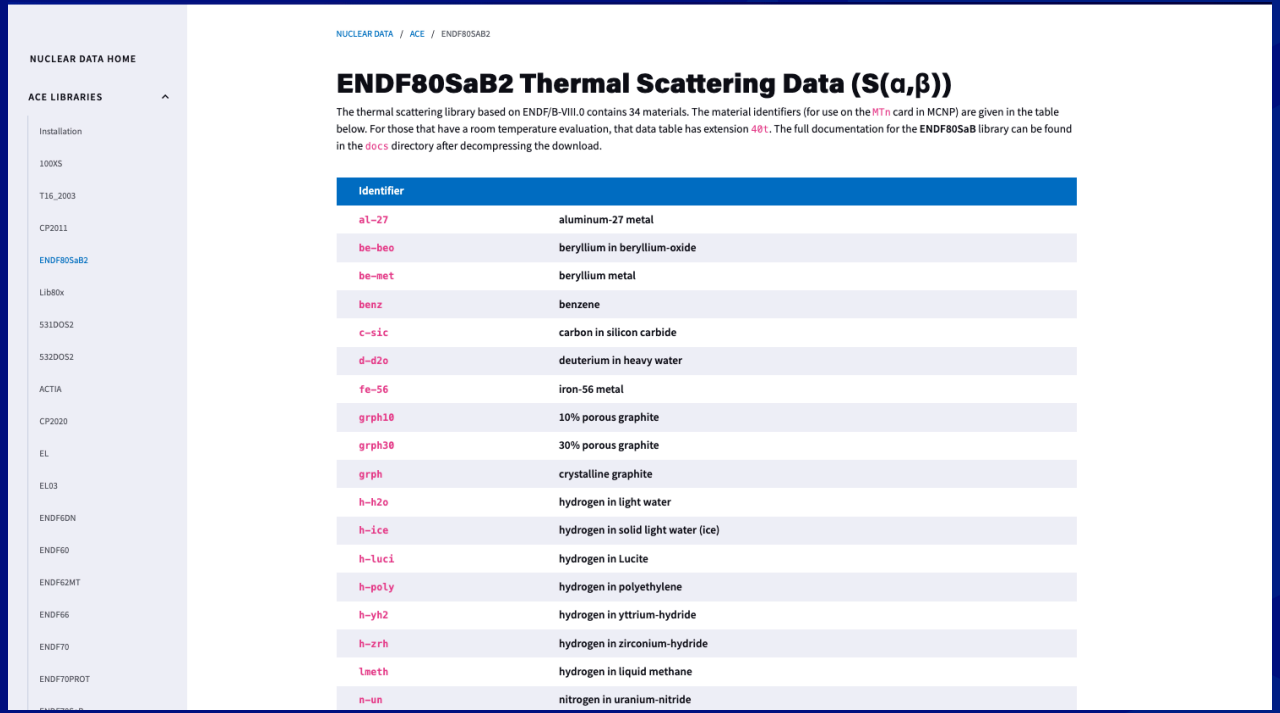
Download

CP2020 can be downloaded either as a zip file or as a compressed tarball

- CP2020.tgz (sha512 `0ffefd530c4dd16afdc755a7abc20f164fcd47d666cd330bfc6c4c1717d8d51`)
- CP2020.zip (sha512 `1fba64f5e7d53e942dd5ed25875511c3ee860e9b5be7bbcffed43bb85d2cb40`)

Future Website Changes

- Faster download speeds
  - Able to download nuclear data before the heat death of the universe



NUCLEAR DATA HOME

ACE LIBRARIES

- Installation
- 100XS
- T16_2003
- CP2011
- ENDF80SaB2
- Lib80x
- 531DOS2
- 532DOS2
- ACTIA
- CP2020
- EL
- EL03
- ENDF6DN
- ENDF60
- ENDF62MT
- ENDF66
- ENDF70
- ENDF70PROT

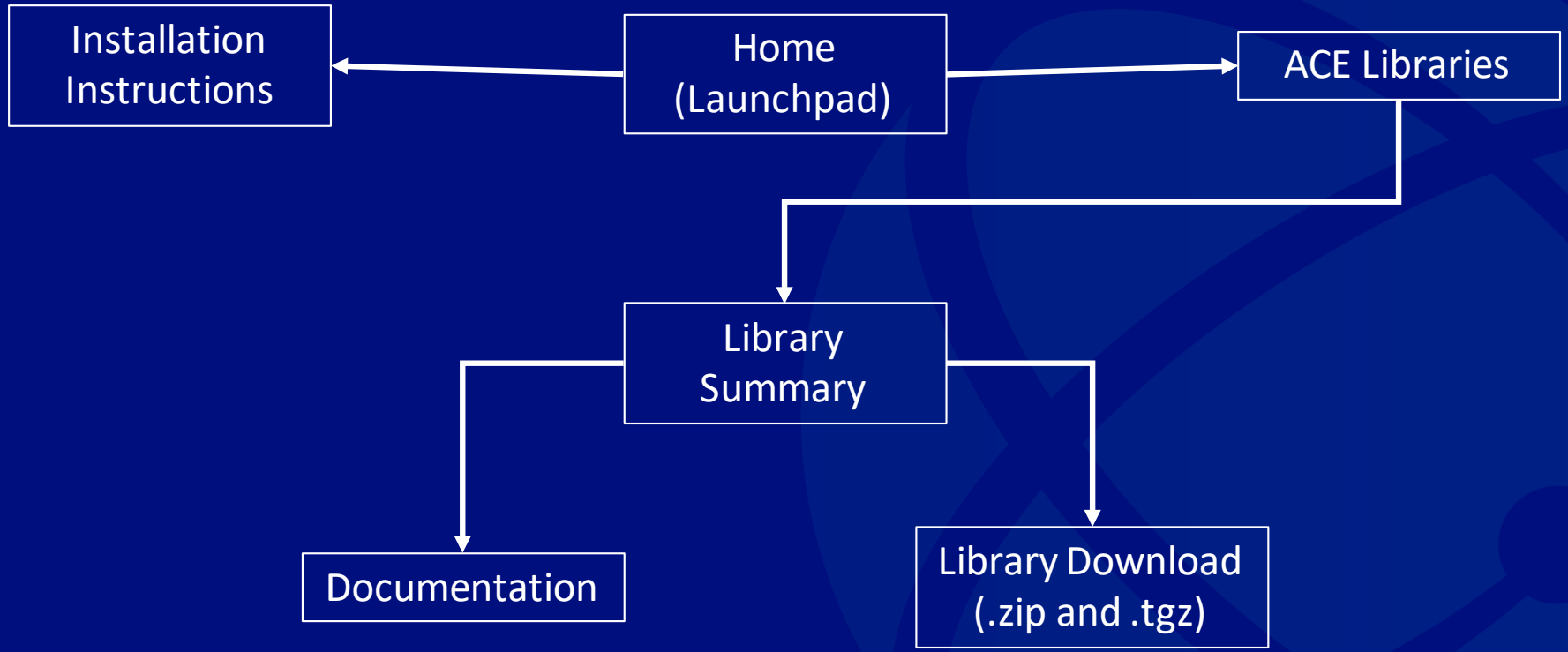
NUCLEAR DATA / ACE / ENDF80SAB2

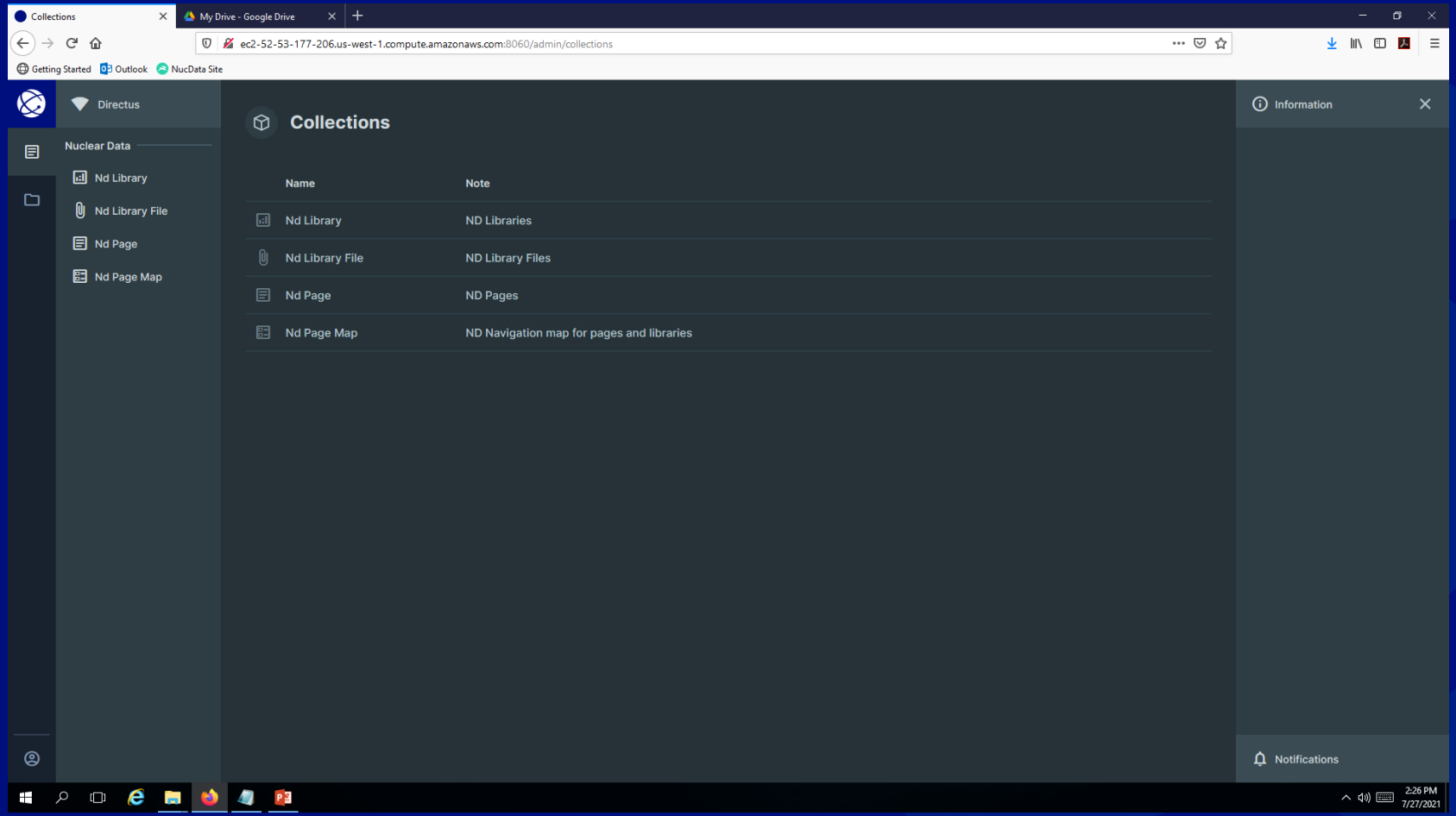
ENDF80SaB2 Thermal Scattering Data (S(α,β))

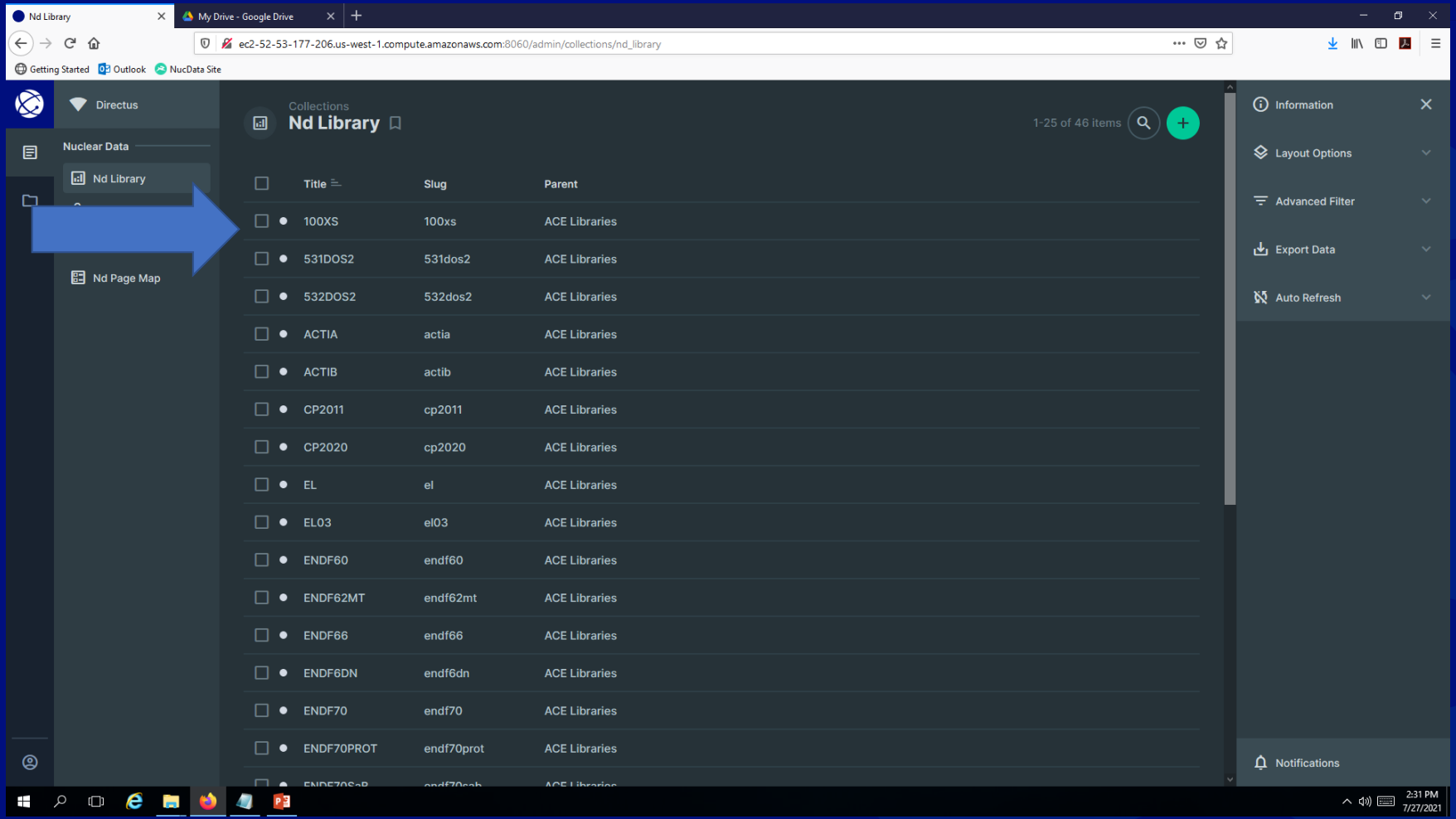
The thermal scattering library based on ENDF/B-VIII.0 contains 34 materials. The material identifiers (for use on the `MTn` card in MCNP) are given in the table below. For those that have a room temperature evaluation, that data table has extension `40t`. The full documentation for the **ENDF80SaB** library can be found in the `docs` directory after decompressing the download.

Identifier	
al-27	aluminum-27 metal
be-beo	beryllium in beryllium-oxide
be-met	beryllium metal
benz	benzene
c-sic	carbon in silicon carbide
d-d2o	deuterium in heavy water
fe-56	iron-56 metal
grph10	10% porous graphite
grph30	30% porous graphite
grph	crystalline graphite
h-h2o	hydrogen in light water
h-ice	hydrogen in solid light water (ice)
h-luci	hydrogen in Lucite
h-poly	hydrogen in polyethylene
h-yh2	hydrogen in yttrium-hydride
h-zrh	hydrogen in zirconium-hydride
lmeth	hydrogen in liquid methane
n-un	nitrogen in uranium-nitride

Website Structure




Collections
My Drive - Google Drive
ec2-52-53-177-206.us-west-1.compute.amazonaws.com:8060/admin/collections
Getting Started
Outlook
NucData Site
Directus
Nuclear Data
Nd Library
Nd Library File
Nd Page
Nd Page Map
Collections
Name
Note
Nd Library
ND Libraries
Nd Library File
ND Library Files
Nd Page
ND Pages
Nd Page Map
ND Navigation map for pages and libraries
Information
Notifications
2:26 PM
7/27/2021


Nd Library
My Drive - Google Drive
ec2-52-53-177-206.us-west-1.compute.amazonaws.com:8060/admin/collections/nd_library
Getting Started
Outlook
NucData Site
Directus
Nuclear Data
Nd Library
Nd Page Map
Collections
Nd Library
1-25 of 46 items
Title
Slug
Parent
100XS 100xs ACE Libraries
531DOS2 531dos2 ACE Libraries
532DOS2 532dos2 ACE Libraries
ACTIA actia ACE Libraries
ACTIB actib ACE Libraries
CP2011 cp2011 ACE Libraries
CP2020 cp2020 ACE Libraries
EL el ACE Libraries
EL03 el03 ACE Libraries
ENDF60 endf60 ACE Libraries
ENDF62MT endf62mt ACE Libraries
ENDF66 endf66 ACE Libraries
ENDF6DN endf6dn ACE Libraries
ENDF70 endf70 ACE Libraries
ENDF70PROT endf70prot ACE Libraries
Information
Layout Options
Advanced Filter
Export Data
Auto Refresh
Notifications
2:31 PM
7/27/2021

Title*

100XS

Slug*

100xs

Parent

ACE Libraries

Body

Editor | Preview

```
# The 100XS Neutron Data Library

The **100xs** library contains 9 data files nuclides each having an  evaluation
extending to 100 MeV. The 9 materials are <sup>9</sup>Be, <sup>12</sup>C,
<sup>16</sup>O, <sup>27</sup>Al, Si, <sup>40</sup>Ca, Fe, W, and <sup>238</sup>U.
Modifications were made to the  original evaluations and resulting data files to
make them more  compatible with MCNP; however, a small patch is necessary for MCNP
4A  for this library. These files have been given the ZAID ending of `.21c`.
Heating numbers on this library are known to overestimate the energy  deposition.

If further information is required contact a member of the Data Team by e-mail at
[nucldata@lanl.gov](mailto:nucldata@lanl.gov)

## Documentation

* "Summary Documentation for the 100XS Neutron Cross Section Library", Little,
R.C, (1995), [la-ur-96-24](http://ec2-52-53-177-206.us-
west-1.compute.amazonaws.com:8060/assets/5c1136b3-9586-4095-adf1-d3ab0cc2ad8b)
```

Description

Patch for MCNP 4A consisting of 9 data files nuclides extending to 100 MeV

Describes library in JSON file

Production*

Enabled

Files

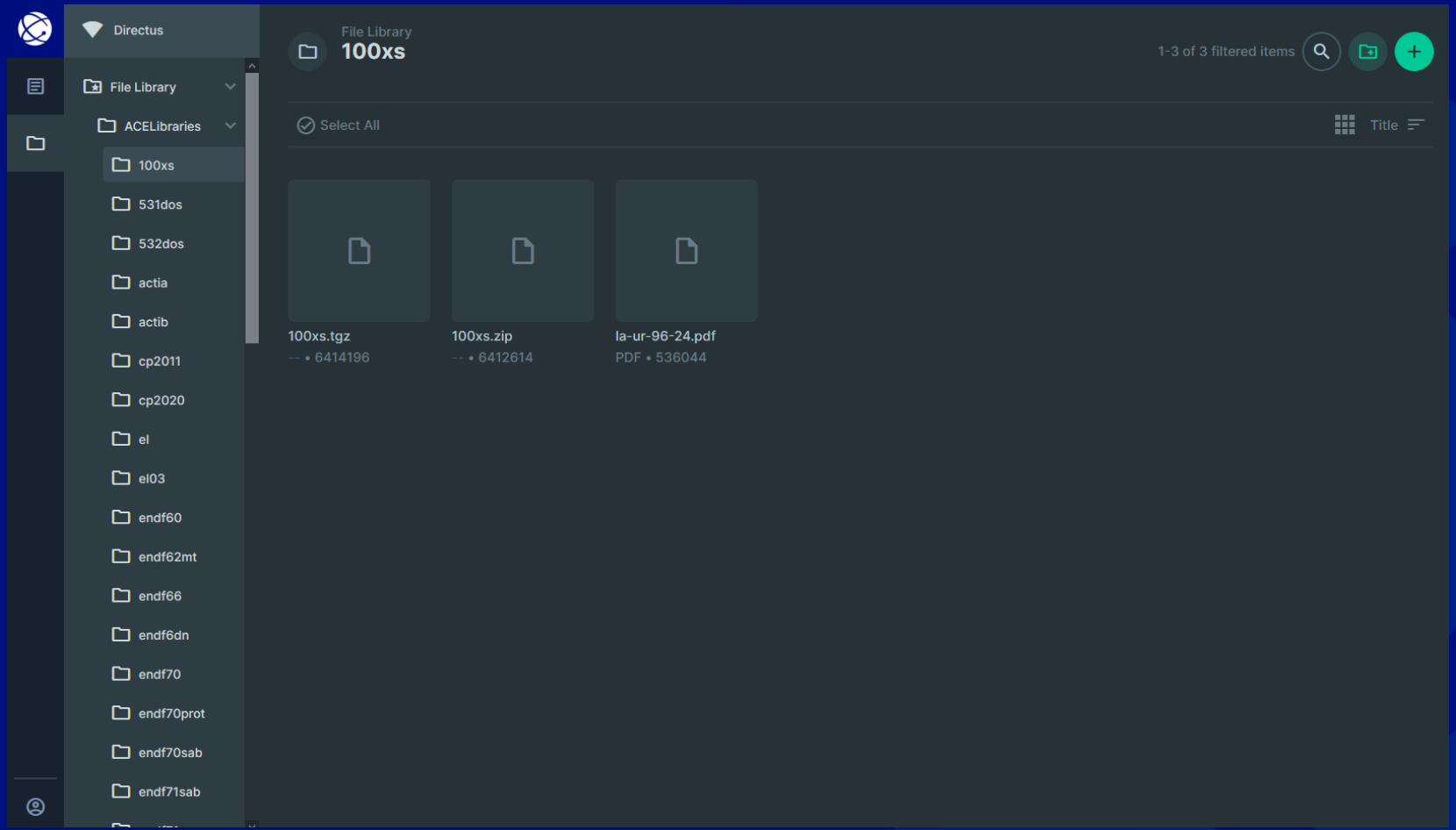
100xs.zip

100xs.tgz

Create New | Add Existing

Sort*

January 1st, 1995 12:00 AM


Directus
File Library
ACELibraries
100xs
531dos
532dos
actia
actib
cp2011
cp2020
el
el03
endf60
endf62mt
endf66
endf6dn
endf70
endf70prot
endf70sab
endf71sab
File Library
100xs
1-3 of 3 filtered items
Select All
Title
100xs.tgz
-- • 6414196
100xs.zip
-- • 6412614
la-ur-96-24.pdf
PDF • 536044

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Questions?

But we're not done ☺

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Tutorial for Generating Correlated Random Samples and Propagation of Uncertainty

Ryan Siggins, Kent Parsons

August 4, 2021

Introduction

- Series of tutorials written by Kent Parsons to generate random variables and manipulate covariances

- Calculated using MATLAB, with tutorials written in Microsoft Word
  - Chock full of information, but can be more accessible

- Move the tutorials to a JupyterLab notebook
  - Keep the information
  - Add code blocks to show examples of the methods in action

Topics

1. Illustrating Uncertainties Without Correlation
2. Illustrating Uncertainties Without Correlation with Negative Samples
3. Illustrating Uncertainties With Correlation
4. Illustrating Uncertainties With a χ-like Constraint
5. Illustrating Uncertainties With a Σ_{tot}-like Constraint
6. Sampling Using Different Distributions
7. Dealing with Negative Eigenvalues in a Covariance Matrix

General Format

$$Y = X_1 + 2X_2 + \frac{X_3}{3} + 5X_4$$

Where each term X_n is defined with a mean and standard deviation

If the samples are correlated, a *correlation* or *covariance* matrix is given

Sandwich Rule

The *Sandwich Rule* calculates the variance of a system if you know the mean and variance of each term

$$V1' = [\frac{dY}{DX_1}, \frac{dY}{DX_2}, \frac{dY}{DX_3}, \frac{dY}{DX_4}]$$

$$V1' * COV * V1 = \sigma^2$$

This gives us something to compare our random samples' analyses to

Can also use the *Relative Sensitivity Vector* and *Relative Covariance Matrix*

Sandwich Rule – Relative Sensitivity Vector and COV

Can also use the *Relative Sensitivity Vector* and *Relative Covariance Matrix*

$$V2' = [\frac{dY}{DX_1} * \mu_1, \quad \frac{dY}{DX_2} * \mu_2, \quad \frac{dY}{DX_3} * \mu_3, \quad \frac{dY}{DX_4} * \mu_4]$$

The *Relative Covariance Matrix* is similar to *COV,* but each term is divided by the product of the related terms' means

$$V2' * RELCOV * V2 = \sigma^2$$

Generating Random Variables

- Use NumPy's built in RNG to produce normal, lognormal, or multivariate normal distributions
  - Simulate collected cross section data to perform analysis on and compare to *Sandwich Rule* results

- From here, we can manipulate the random distributions to improve our results

Tutorials Demo

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Questions?

The end for real this time ☺